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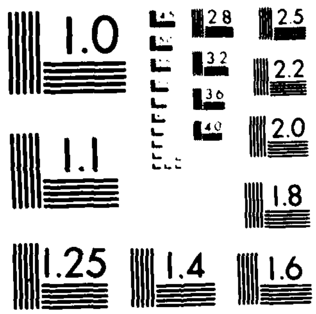

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THE NUMBER OF SOLUTIONS OF AN EQUATION FROM CATALYSIS

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THE NUMBER OF SOLUTIONS OF AN EQUATION FROM CATALYSIS

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ABSTRACT

In catalysis theory there is interest in the number of solutions of the equation

$$v'' + \lambda(1 + \beta - v)^p e^{-\gamma/v} ,$$

with the boundary conditions

$$v'(0) = 0, \quad v(1) = 1 ,$$

the parameters λ, β, γ being all positive and p a non-negative integer. The paper answers this question when γ is large, which is the interesting situation physically, and although the treatment is somewhat different in the cases $p = 0$ and $p \neq 0$, the final answer is the same, that, given β, there exist two positive functions $\lambda_1(\gamma)$ and $\lambda_2(\gamma)$ such that the problem has one solution if $\lambda < \lambda_1(\gamma)$ or $\lambda > \lambda_2(\gamma)$, three solutions if $\lambda_1(\gamma) < \lambda < \lambda_2(\gamma)$, and two solutions if $\lambda = \lambda_1(\gamma)$ or $\lambda = \lambda_2(\gamma)$.

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Work Unit Number 1 (Applied Analysis)

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SIGNIFICANCE AND EXPLANATION

In the production of chemicals, catalysts are often required to convert gaseous reactants into useful products. Frequently the catalyst is in the form of a porous pellet and the gas must diffuse into the interior of the pellet so that the catalyst there is fully utilized. Depending upon the relative rates of diffusion and reaction, temperature and concentration gradients are set up across the pellet, and their determination is essential for the calculation of the over-all rate of conversion. The modelling of these processes within the pellet leads to a set of parabolic partial differential equations, and a first step in the study of these is to determine whether there exist steady-state solutions, and, if so, how many of these there are.

The present paper works at a particular one-dimensional steady-state equation which nonetheless seems to be typical of more general situations, and it is shown rigorously that if the activation energy is sufficiently high, then the number of solutions must be essentially either one or three (depending upon the other parameters in the problem).

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The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

THE NUMBER OF SOLUTIONS OF AN EQUATION FROM CATALYSIS

S. P. Hastings and J. B. McLeod

1. INTRODUCTION

We are interested in the number of solutions of the equation

(1.1) $$v'' + \lambda(1 + \beta - v)^p e^{-\gamma/v} ,$$

with the boundary conditions

(1.2) $$v'(0) = 0, \quad v(1) = 1 .$$

This is the one-dimensional case of an equation of some importance in catalysis theory, the parameters λ, β, γ being all positive, and p a non-negative integer. Readers interested in the derivation of the equation and its physical interpretation are referred to the work by Aris [1], particularly section 2.5.4.

Relevant work on the analysis of this problem has been done by Dancer [2] and Parter [3]. Dancer's work is concerned with the case $p = 1$, although he mentions that it can be extended to other values of p, and he shows that, with β fixed and γ large, there are at most three solutions of the problem except for a relatively small range of values of λ where he is unable to come to any conclusion. His argument, which depends upon regarding (1.1) as a perturbation of the Gelfand equation

$$u'' + \mu e^u = 0$$

and using ideas from bifurcation theory, extends also to radially symmetric solutions in two dimensions, and he shows that the problem is fundamentally different in higher dimensions still, in that, for γ large, there may be values of λ giving large numbers of solutions. His work in one and two dimensions is therefore a partial answer to the conjecture that in these dimensions the problem has at most three solutions.

Parter is concerned with two dimensions and an equation which is a generalisation of the case $p = 0$. His results delineate a region of the parameter space in which there exist at least three solutions, and another in which there exists at most one.

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Our results are more similar to those of Dancer, although obtained in quite a different way. The restriction to one dimension arises because we intend to use the autonomous nature of the equation in that case to reduce the problem to an integration, and we can then establish that for (1.1) with $p = 0$ and the boundary data

$$v'(0) = 0, \quad v(1) = 0 , \tag{1.3}$$

the problem has either two solutions or none, this regardless of whether or not γ is large. (Given γ, there is one exceptional value of λ for which the two solutions become coincident.) The introduction of the boundary condition $v(1) = 1$ can be regarded, at least for large γ, as a perturbation, and by studying this perturbation we are able to assert that (1.1)-(1.2) has, if γ is sufficiently large, either one solution or three (except for two exceptional values of λ where there are two). Unlike the Dancer result, there is no restriction on λ. There would seem little doubt that the result remains true whether γ is large or not, but the analysis required for its proof seems too formidable.

Our approach is similar in spirit to that of Smoller and Wasserman [4], who studied the number of solutions of another autonomous problem by reducing it to an integral. Their nonlinearity was cubic, however, resulting in completely different analysis.

For $p \neq 0$, and boundary data (1.3), we establish again that there are either two solutions or none, although, in contrast with the case $p = 0$, we have to assume γ large in order to assert this. This in turn leads to the same result as for $p = 0$ with the original boundary conditions (1.2), namely that for γ large there is either one solution or three, except at two transitional values of λ where there are two.

There is a variant of the problem, still of physical interest, in which the equation is replaced by

$$v'' + \lambda\{\beta + \frac{\mu}{\nu} + v(1)(1 - \frac{\mu}{\nu}) - v\}^p e^{-\gamma/v} = 0 ,$$

with the boundary conditions

$$v'(0) = 0, \quad v'(1) = \mu\{1 - v(1)\} ,$$

μ, ν positive. This has been studied by Kapila and Matkowsky [5], and also by D. G. Schaeffer [private communication], who show that the perturbation corresponding to changing from (1.3) to (1.2) can produce two further solutions, so that there can be from one to

five. This problem is not studied in the present paper, although there would seem to be no reason why the methods used here should not extend.

The arguments would certainly allow us to alter the nonlinearity $e^{-\gamma/v}$ to something more general, but there does seem to be a large measure of agreement that $e^{-\gamma/v}$ is the correct nonlinearity, and so no attempt has been made to push the theorems in the direction of generalisation.

In §2 we prove the basic theorem for (1.1) and (1.3) with $p = 0$, and carry out the perturbation to (1.2) in §3. Later sections deal with the case $p > 0$.

2. THE CASE $p = 0$ WITH ZERO BOUNDARY DATA

We are interested in the boundary-value problem

$$v'' + \lambda e^{-\gamma/v} = 0 \,, \tag{2.1}$$

$$v'(0) = 0, \quad v(1) = 0 \,. \tag{2.2}$$

Since $\lambda > 0$, and the exponential is non-negative, we must have $v'' < 0$, and so $v' < 0$, $v(0) > 0$. Set

$$v = \alpha Y \,,$$

where α is so chosen that

$$Y(0) = 1 \,.$$

The equation for Y is

$$\alpha \frac{d^2Y}{dx^2} + \lambda e^{-\gamma/\alpha Y} = 0 \,.$$

Set

$$x = \alpha^{1/2}X, \quad Y' = dY/dX \,,$$

and we have

$$Y'' = \lambda e^{-\gamma/\alpha Y} = 0 \,,$$

$$Y(0) = 1, \quad y'(0) = 0, \quad Y(\alpha^{-1/2}) = 0 \,.$$

Thus

$$Y'^2 = -2\lambda \int_1^Y e^{-\gamma/\alpha t} dt \,,$$

$$\frac{dX}{dY} = -(2\lambda)^{-1/2}\left(\int_Y^1 e^{-\gamma/\alpha t} dt\right)^{-1/2} \,,$$

and integration with respect to Y over $[0,1]$ gives

$$\alpha^{-1/2} = (2\lambda)^{-1/2} \int_0^1 \left(\int_Y^1 e^{-\gamma/\alpha t} dt\right)^{-1/2} dY \,, \tag{2.3}$$

or, with $\gamma = \alpha\mu$,

$$(2.4) \qquad \left(\frac{2\lambda}{\gamma}\right)^{1/2} = \mu^{-1/2} \int_0^1 \left(\int_Y^1 e^{-\mu/t} dt\right)^{-1/2} dY .$$

Now our object is to show that, given λ, γ, there exist at most two solutions α of (2.3), *or*, equivalently, at most two solutions μ of (2.4), for, through $v(0) = \alpha$, two solutions for α means two solutions for our original boundary-value problem. What we shall actually prove, and it clearly implies the above, is

<u>Theorem 1</u>. <u>For</u> $\mu > 0$, <u>define</u> $f(\mu)$ <u>by</u>

$$f(\mu) = \mu^{-1/2} \int_0^1 \left(\int_Y^1 e^{-\mu/t} dt\right)^{-1/2} dY .$$

<u>Then</u> $f'(\mu)$ <u>has precisely one zero, and that simple.</u>

<u>Proof</u>. Let $F(u) = e^{-u}$. Then

$$(2.5) \qquad \mu \frac{df}{d\mu} = -\frac{1}{2} f - \frac{1}{2} \mu^{1/2} \int_0^1 \frac{\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right) dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right) dt\right\}^{3/2}} dY .$$

Since $F' = -F$, and $t \leq 1$ in the ranges of integration, we see that

$$(2.6) \qquad \int_Y^1 F\left(\frac{\mu}{t}\right) dt \leq -\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right) dt ,$$

and so

$$\mu \frac{df}{d\mu} > -\frac{1}{2} f + \frac{1}{2} \mu f .$$

Hence $f'(\mu) > 0$ if $\mu > 1$, and we need concern ourselves only with $\mu < 1$. Then

$$\left(\mu \frac{d}{d\mu}\right)^2 f = -\frac{1}{2}\mu \frac{df}{d\mu} - \frac{1}{4}\mu^{1/2}\int_0^1 \frac{\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\, dY$$

$$+ \frac{3}{4}\mu^{3/2}\int_0^1 \frac{\left\{\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt\right\}^2}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{5/2}}\, dY - \frac{1}{2}\mu^{3/2}\int_0^1 \frac{\int_Y^1 \frac{1}{t^2} F''\left(\frac{\mu}{t}\right)dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\, dY \ .$$

But

$$\int_Y^1 \frac{1}{t^2} F''\left(\frac{\mu}{t}\right)dt = -\frac{1}{\mu}\left\{F'(\mu) - F'\left(\frac{\mu}{Y}\right)\right\} < -\frac{1}{\mu}\left\{F'(\mu) - YF'\left(\frac{\mu}{Y}\right)\right\} , \tag{2.7}$$

$$\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt = -\frac{1}{\mu}\left\{F(\mu) - YF\left(\frac{\mu}{Y}\right)\right\} + \frac{1}{\mu}\int_Y^1 F\left(\frac{\mu}{t}\right)dt , \tag{2.8}$$

so that

$$\int_Y^1 \frac{1}{t^2} F''\left(\frac{\mu}{t}\right)dt < -\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt + \frac{1}{\mu}\int_Y^1 F\left(\frac{\mu}{t}\right)dt ,$$

and

$$\left(\mu \frac{d}{d\mu}\right)^2 f > -\frac{1}{2}\mu \frac{df}{d\mu} - \frac{1}{4}\mu^{1/2}\int_0^1 \frac{\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\, dY$$

$$+ \frac{3}{4}\mu^{3/2}\int_0^1 \frac{\left\{\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt\right\}^2}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{5/2}}\, dY + \frac{1}{2}\mu^{3/2}\int_0^1 \frac{\int_Y^1 \frac{1}{t} F'\left(\frac{\mu}{t}\right)dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\, dY - \frac{1}{2}\mu f \ .$$

When $\frac{df}{d\mu} = 0$, we can use (2.5) to obtain

$$\mu^2 \frac{d^2f}{d\mu^2} = -\frac{1}{4}\mu^{1/2}\int_0^1 \frac{\int_Y^1 \frac{1}{t}F'\left(\frac{\mu}{t}\right)dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\,dY$$

$$+\frac{3}{4}\mu^{3/2}\int_0^1 \frac{\left\{\int_Y^1 \frac{1}{t}F'\left(\frac{\mu}{t}\right)dt\right\}^2}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{5/2}}\,dY + \mu^{3/2}\int_0^1 \frac{\int_Y^1 \frac{1}{t}F'\left(\frac{\mu}{t}\right)dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\,dY$$

$$> \left(\frac{1}{4}\mu^{1/2} + \frac{3}{4}\mu^{3/2} - \mu^{3/2}\right)\int_0^1 \frac{\int_Y^1 \frac{1}{t}\left|F'\left(\frac{\mu}{t}\right)\right|dt}{\left\{\int_Y^1 F\left(\frac{\mu}{t}\right)dt\right\}^{3/2}}\,dY ,$$

from (2.6). Hence, with $\mu < 1$, $f'(\mu) = 0$ implies $f''(\mu) > 0$, and so $f'(\mu)$ has at most one zero, and that simple.

It remains to be proved that f' does possess one zero. However for small μ we have

$$f(\mu) \sim 2\mu^{-1/2}, \quad f'(\mu) \sim -\mu^{-3/2} ,$$

and we have already seen that $f'(\mu) > 0$ for $\mu > 1$, so that certainly $f'(\mu)$ has a zero.

The following result is an immediate corollary of Theorem 1.

<u>Theorem 2</u>. <u>For the boundary-value problem (2.1)-(2.2), there exists a positive number</u> K <u>such that the problem has no solution if</u> $\lambda/\gamma < K$, <u>just one solution if</u> $\lambda/\gamma = K$, <u>and two solutions if</u> $\lambda/\gamma > K$.

3. THE CASE $p = 0$ WITH NON-ZERO BOUNDARY DATA

We now consider

$$v'' + \lambda e^{-\gamma/v} = 0 \,, \tag{3.1}$$

$$v'(0) = 0, \quad v(1) = 1 \,. \tag{3.2}$$

With the same substitutions as in §2, this reduces to

$$Y'' + \lambda e^{-\gamma/\alpha Y} = 0 \,,$$

$$Y(0) = 1, \quad Y'(0) = 0, \quad Y(\alpha^{-1/2}) = \alpha^{-1}, \quad \alpha > 1 \,,$$

which in turn leads to

$$\alpha^{-1/2} = (2\lambda)^{-1/2} \int_{\alpha^{-1}}^{1} \Big(\int_{Y}^{1} e^{-\gamma/\alpha t} dt\Big)^{-1/2} dY \,,$$

or, with $\gamma = \alpha\mu$, to

$$\Big(\frac{2\lambda}{\gamma}\Big)^{1/2} = \mu^{-1/2} \int_{\mu/\gamma}^{1} \Big\{\int_{Y}^{1} e^{-\mu/t} dt\Big\}^{-1/2} dY \,.$$

Let us now define

$$f_1(\mu) = \mu^{-1/2} \int_{\mu/\gamma}^{1} \Big\{\int_{Y}^{1} e^{-\mu/t} dt\Big\}^{-1/2} dY \,.$$

We are interested only in γ large, and then $f_1(\mu)$ behaves like $f(\mu)$ in Theorem 1 except when μ also is large. In particular, there is an $\varepsilon > 0$ such that, if γ is sufficiently large, then on the interval $0 < \mu \le \varepsilon\gamma$, $f_1(\mu)$ first decreases to a minimum, and then increases. On the other hand, while $f(\mu)$ is defined for all $\mu > 0$, with $f(\mu) \to \infty$ as $\mu \to \infty$, $f_1(\mu)$ makes sense only for $\mu \le \gamma$, and $f_1(\gamma) = 0$. Our goal is to show that (3.1)-(3.2) has at most three solutions, as stated in Theorem 4 below, and this is a clear consequence of

Theorem 3. *For γ sufficiently large, $f_1'(\mu)$ has precisely two zeros in the range $0 < \mu \le \gamma$, and those are simple. One occurs close to the zero of $f'(\mu)$, and the other with*

$$\mu = \gamma - 2 \log x_0 + O(\gamma^{-1} \log \gamma) \,,$$

where x_0 is the unique root exceeding 1 of

$$\cosh^{-1}x = x/(x^2 - 1)^{1/2} . \tag{3.3}$$

(That there is a unique root exceeding 1 of (3.3) follows by considering the difference of the two sides, recalling that

$$\frac{d}{dx}\cosh^{-1}x = (x^2 - 1)^{-1/2} .)$$

<u>Theorem 4. If</u> γ <u>is sufficiently large in the boundary-value problem (3.1)-(3.2), then there exist two positive functions</u> $K_1(\gamma)$, $K_2(\gamma)$ <u>such that the problem has one solution if</u> $\lambda < K_1(\gamma)$ <u>or</u> $\lambda > K_2(\gamma)$, <u>three solutions if</u> $K_1(\gamma) < \lambda < K_2(\gamma)$, <u>and two solutions if</u> $\lambda = K_1(\gamma)$ <u>or</u> $\lambda = K_2(\gamma)$.

<u>Proof of Theorem 3.</u>

Making the changes of variable

$$t = \mu z, \quad Y = \mu Z, \quad z = u^{-1}, \quad Z = U^{-1} ,$$

we have

$$f_1(\mu) = \int_{1/\gamma}^{1/\mu} \{\int_Z^{1/\mu} e^{-1/z}dz\}^{-1/2}dZ , \tag{3.4}$$

and

$$\int_Z^{1/\mu} e^{-1/z}dz = e^{-\mu}\int_Z^{1/\mu} e^{\mu-1/z}dz$$

$$= e^{-\mu}\int_\mu^U \frac{1}{u^2} e^{\mu-u}du = e^{-\mu}\int_0^{U-\mu} \frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta .$$

Now, by integration by parts,

$$\int_0^{U-\mu} \frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta = \left(\frac{1}{\mu^2} - \frac{e^{\mu-U}}{U^2}\right) - 2\int_0^{U-\mu} \frac{e^{-\theta}}{(\theta+\mu)^3}\,d\theta ,$$

so that

$$\int_0^{U-\mu} \frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta\{1 + F(\mu,U)\} = \frac{1}{\mu^2} - \frac{e^{\mu-U}}{U^2} , \tag{3.5}$$

where

$$f(\mu,U) = 2\int_0^{U-\mu} \frac{e^{-\theta}}{(\theta+\mu)^3}\,d\theta \Big/ \int_0^{U-\mu} \frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta .$$

It is clear that

$$(3.6) \qquad f(\mu,U) < 2\mu^{-1} ,$$

but we can also assert that, for large μ,

$$(3.7) \qquad \frac{\partial F}{\partial \mu}(\mu,U) = O(\mu^{-2}) ,$$

uniformly in U for $\mu \le U \le \gamma$. (We recall that we are only interested in large μ, since $f_1(\mu)$ behaves like $f(\mu)$ when μ is not large.) The truth of (3.7) is obvious so far as those terms in the differentiation are concerned which arose from differentiation under the integral signs. The terms arising from differentiating the limits of integration are (omitting a factor 2)

$$\left\{-\frac{e^{\mu-U}}{U^3}\int_0^{U-\mu}\frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta + \frac{e^{\mu-U}}{U^2}\int_0^{U-\mu}\frac{e^{-\theta}}{(\theta+\mu)^3}\,d\theta\right\} \Big/ \left\{\int_0^{U-\mu}\frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta\right\}^2$$

$$= \frac{e^{\mu-U}}{U^3}\int_0^{U-\mu}\frac{e^{-\theta}}{(\theta+\mu)^3}(U-\mu-\theta)\,d\theta \Big/ \left\{\int_0^{U-\mu}\frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta\right\}^2 .$$

If $U - \mu \le 1$, then the numerator does not exceed

$$\mu^{-6}\int_0^{U-\mu}(U-\mu-\theta)\,d\theta = \frac{1}{2}\mu^{-6}(U-\mu)^2 ,$$

while the denominator is not less then

$$\left(\frac{e^{\mu-U}}{U^2}\int_0^{U-\mu}d\theta\right)^2 \ge K\mu^{-4}(U-\mu)^2$$

for some constant K, since $U - \mu \le 1$. Thus (3.7) follows if $U - \mu \le 1$. If $U - \mu \ge 1$, the numerator does not exceed

$$\mu^{-6}(U-\mu)e^{\mu-U}\int_0^{\infty} e^{-\theta}\,d\theta \le e^{-1}\mu^{-6} ,$$

while the denominator is not less than

$$\left\{\int_0^{1}\frac{e^{-\theta}}{(\theta+\mu)^2}\,d\theta\right\}^2 \ge \frac{e^{-2}}{(\mu+1)^4} .$$

Hence again (3.7) follows.

From (3.4), (3.5), (3.6),

$$f_1(\mu) = e^{\frac{1}{2}\mu} \int_{\mu}^{\gamma} \frac{1}{U^2} \left(\frac{1}{\mu^2} - \frac{e^{\mu-U}}{U^2} \right)^{-1/2} \{1 + O(\mu^{-1})\} dU$$

$$= e^{\frac{1}{2}\mu} \int_{\mu}^{\gamma} \frac{\mu U^{-1} e^{\frac{1}{2}U}}{(U^2 e^U - \mu^2 e^{\mu})^{1/2}} \{1 + O(\mu^{-1})\} dU$$

$$= e^{\frac{1}{2}\mu} \int_{\mu e^{\frac{1}{2}\mu}}^{\gamma e^{\frac{1}{2}\gamma}} \frac{2\mu U^{-2}}{(x^2 - \mu^2 e^{\mu})^{1/2}} \{1 + O(\mu^{-1})\} dx ,$$

where $x = Ue^{\frac{1}{2}U}$ and the O-term, thanks to (3.7), has the property that, if differentiated with respect to μ, it yields $O(\mu^{-2})$. Thus, with $x = \mu e^{\frac{1}{2}\mu} t$,

$$f_1(\mu) = e^{\frac{1}{2}\mu} \int_{1}^{\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu}} \frac{2\mu U^{-2}}{(t^2 - 1)^{1/2}} \{1 + O(\mu^{-1})\} dt . \tag{3.8}$$

If $\mu > \gamma - \log \gamma$, then $U = \mu + O(\log \mu)$, and so

$$f_1(\mu) = 2\mu^{-1} e^{\frac{1}{2}\mu} \int_{1}^{\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu}} (t^2 - 1)^{-1/2} \{1 + O(\mu^{-1} \log \mu)\} dt$$

$$= 2\mu^{-1} e^{\frac{1}{2}\mu} \cosh^{-1}(\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu}) \{1 + O(\mu^{-1} \log \mu)\} ,$$

our previous remarks about differentiating the O-term implying now that differentiation of the last O-term will yield $O(\mu^{-2} \log \mu)$. Thus

$$f_1'(\mu) = \{\tfrac{1}{2} + O(\mu^{-1})\}f_1(\mu)$$

$$+ 2\mu^{-1}e^{\frac{1}{2}\mu}\left(\frac{\gamma^2 e^{\gamma}}{\mu^2 e^{\mu}} - 1\right)^{-1/2}\left(-\frac{\gamma e^{\frac{1}{2}\gamma}}{\mu^2 e^{\mu}}\right)e^{\frac{1}{2}\mu}\left(\tfrac{1}{2}\mu + 1\right)\{1 + O(\mu^{-1}\log\mu)\} ,$$

and so $f_1'(\mu) = 0$ when

$$\cosh^{-1}(\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu}) = \frac{\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu}}{\left(\frac{\gamma^2 e^{\gamma}}{\mu^2 e^{\mu}} - 1\right)^{1/2}}\{1 + O(\mu^{-1}\log\mu)\} ,$$

i.e. when

$$\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu} = x_0 + O(\mu^{-1}\log\mu) ,$$

where x_0 is defined in the statement of the theorem. Thus

$$\mu = \gamma - 2\log x_0 + O(\gamma^{-1}\log\gamma) .$$

We are now assured that there is a root of $f_1'(\mu)$ with $\mu > \gamma - \log\gamma$, and that it necessarily satisfies (3.9). To prove that there is just one, and that one simple, we evaluate $f_1''(\mu)$ with μ satisfying (3.9) and show that $f_1''(\mu) < 0$. (We leave the straightforward calculations to the reader.) We can also use (3.8) in similar manner to prove that $f_1'(\mu) > 0$ if $\epsilon\gamma < \mu < \gamma - \log\gamma$, and the proof of Theorem 3 is complete.

4. THE CASE $p \neq 0$ WITH ZERO BOUNDARY DATA

We are interested in the problem

$$v'' + \lambda(1 + \beta - v)^p e^{-\gamma/v} ,$$

with

$$v'(0) = 0, \quad v(1) = 0 ,$$

and we are interested in solutions for which $v < 1 + \beta$. As in §2, we set

$$v = \alpha Y, \quad x = \alpha^{1/2} X ,$$

where

$$Y(0) = 1, \quad \alpha = v(0) < 1 + \beta .$$

The equation for Y $(Y' = dY/dX)$ is

$$Y'' + \lambda(1 + \beta - \alpha Y)^p e^{-\gamma/\alpha Y} = 0 ,$$

$$Y(0) = 1, \quad Y'(0) = 0, \quad Y(\alpha^{-1/2}) = 0 .$$

Thus

$$\alpha^{-1/2} = (2\lambda)^{-1/2} \int_0^1 \left(\int_Y^1 (1 + \beta - \alpha t)^p e^{-\gamma/\alpha t} dt\right)^{-1/2} dY ,$$

or, with $\gamma = \alpha\mu$, $\alpha < 1 + \beta$, $\mu > \gamma/(1 + \beta)$,

$$\left(\frac{2\lambda}{\gamma}\right)^{1/2} = \mu^{-1/2} \int_0^1 \left[\int_Y^1 (1 + \beta - \gamma t/\mu)^p e^{-\mu/t} dt\right]^{1/2} dY . \tag{4.2}$$

Given λ, γ, we want to show that there exist at most two solutions α of (4.1), or at most two solutions μ of (4.2). We shall actually prove

Theorem 5. *For $\mu > \gamma/(1 + \beta)$ define $g(\mu)$ by*

$$g(\mu) = \mu^{-1/2} \int_0^1 \left(\int_Y^1 (1 + \beta - \gamma t/\mu)^p e^{-\mu/t} dt\right)^{-1/2} dY .$$

Then for γ sufficiently large, β fixed, $g'(\mu)$ has precisely one zero, and that simple. Further, for this zero, μ is close to $\gamma/(1 + \beta)$, being given more precisely by (4.9) or (4.10) below.

Proof. For convenience, write

$$K = (1 + \beta)/\gamma, \quad t = \mu/u, \quad Y = \mu/T ,$$

and we have

$$\gamma^{\frac{1}{2}p} g(\mu) = \int_{\mu}^{\infty} T^{-2}\left\{\int_{\mu}^{T} u^{-2}\left(K - \frac{1}{u}\right)^p e^{-u} du\right\}^{-1/2} dT .$$

With

$$u = \theta + \mu, \quad T = \sigma + \mu ,$$

we have

$$\gamma^{\frac{1}{2}p} g(\mu) = \int_{0}^{\infty} (\mu + \sigma)^{-2}\left\{\int_{0}^{\sigma} (\mu + \theta)^{-2}\left(K - \frac{1}{\mu + \theta}\right)^p e^{-\mu-\theta} d\theta\right\}^{-1/2} d\sigma$$

$$= K^{-\frac{1}{2}p} e^{\frac{1}{2}\mu} \int_{0}^{\infty} (\mu + \sigma)^{-2}\left\{\int_{0}^{\sigma} \frac{(\mu + \theta - K^{-1})^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta\right\}^{-1/2} d\sigma ,$$

i.e.

$$G(\mu) = e^{\frac{1}{2}\mu} \int_{0}^{\infty} (\mu + \sigma)^{-2}\left\{\int_{0}^{\sigma} \frac{(\mu + \theta - K^{-1})^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta\right\}^{-1/2} d\sigma , \tag{4.3}$$

where $G(\mu) = (K\gamma)^{\frac{1}{2}p} g(\mu)$.

We shall show that $G'(\mu)$ (or equivalently $g'(\mu)$) can be zero only if $\mu - K^{-1}$ is small, and we first investigate the inner integral in (4.3). For convenience, we write

$$a = \mu - K^{-1} ,$$

and then the inner integral is

$$\int_{0}^{\sigma} \frac{(a + \theta)^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta = e^{a} \int_{a}^{a+\sigma} \frac{\tau^p e^{-\tau}}{(\mu + \tau - a)^{p+2}} d\tau . \tag{4.4}$$

To deal first with a large, we note that if we differentiate $G(\mu)$, we can differentiate $e^{\frac{1}{2}\mu}$ (which merely multiplies by 1/2), or we can differentiate $(\mu + \sigma)^{-2}$ (which multiplies by a factor $O(\mu^{-1})$), or we can differentiate the inner integral. Differentiating the left-hand expression in (4.4) under the integral sign, we see that we

collect a factor $O(a^{-1})$ or $O(\mu^{-1})$, and so when we differentiate $G(\mu)$ we similarly collect such a factor, and so the leading term in the derivative is that arising from the differentiation of $e^{\frac{1}{2}\mu}$, and $G'(\mu) > 0$.

To deal next with the case where a is moderate, we see that

$$(4.5) \qquad \begin{cases} (4.4) \asymp \sigma a^p \mu^{-(p+2)} & \text{if } \sigma < \Lambda , \\ (4.4) e^{-a} \asymp \mu^{-(p+2)} \int_a^\infty \tau^p e^{-\tau} d\tau & \text{if } \sigma > \Lambda , \end{cases}$$

where Λ is a fixed number chosen so that

$$(a + \sigma)^p e^{-(a+\sigma)} < a^p e^{-a} \quad \text{for} \quad \sigma > \Lambda ,$$

and $\asymp$ means that each side is bounded by a positive constant times the other as $\mu \to \infty$. We remark also that if we differentiate (4.4) (with respect to μ), then we see that the order relations obtained by formally differentiating (4.5) are valid. (This uses the choice of Λ.) Thus

$$G(\mu) \asymp e^{\frac{1}{2}\mu} \mu^{\frac{1}{2}p+1} \{a^{-\frac{1}{2}p} \int_0^\Lambda (\mu + \sigma)^{-2} \sigma^{-1/2} d\sigma + e^{-\frac{1}{2}a} \mu^{-1} (\int_a^\infty \tau^p e^{-\tau} d\tau)^{-1/2}\}$$

$$\asymp e^{\frac{1}{2}\kappa^{-1}} \mu^{\frac{1}{2}p} (\int_a^\infty \tau^p e^{-\tau} d\tau)^{-1/2} .$$

In view of the remark just made about differentiation, we can differentiate this last order relation, whence it is clear that $G'(\mu) > 0$.

We know therefore that a must be small for $G'(\mu) = 0$. To determine a more precisely, we write

$$G(\mu) = e^{\frac{1}{2}\mu} \{\int_0^\varepsilon + \int_\varepsilon^\Lambda + \int_\Lambda^\infty\} (\mu + \sigma)^{-2} \{\int_0^\sigma \frac{(a + \theta)^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta\}^{-1/2} d\sigma$$

$$= G_1(\mu) + G_2(\mu) + G_3(\mu) ,$$

say, where ε is a small fixed positive number, and Λ a large one, both independent of

μ. Then

$$G_1(\mu) = e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}\{1+O(\mu^{-1})\}\{1+O(\varepsilon)\}\int_0^{\varepsilon}\left\{\frac{1}{p+1}\left[(a+\sigma)^{p+1}-a^{p+1}\right]\right\}^{-1/2}d\sigma$$

$$= (p+1)^{1/2}e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}a^{\frac{1}{2}-\frac{1}{2}p}\int_0^{\varepsilon/a}\left\{(\phi+1)^{p+1}-1\right\}^{-1/2}d\phi\{1+O(\mu^{-1})\}\{1+O(\varepsilon)\} .$$

The integral in the last formula line converges, to C_p, say, as $\mu \to \infty$ and $a \to 0$, ε being fixed, provided that $p > 1$. If $p = 1$, it is asymptotic to

$$\log \varepsilon - \log a .$$

It is easy to verify that formal differentiation of the asymptotic expression for G_1 is justified, and that the major contribution to G_1' comes from the differentiation of factors involving a. Thus, for $p > 1$,

$$G_1'(\mu) = \frac{1}{2}(p+1)^{1/2}(1-p)e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}a^{-\frac{1}{2}(p+1)}\int_0^{\varepsilon/a}\left\{(\phi+1)^{p+1}-1\right\}^{-1/2}d\phi \times$$

$$\times\{1+O(\mu^{-1})\}\{1+O(\varepsilon)\}\{1+O(a)\}$$

$$-(p+1)^{1/2}e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}a^{\frac{1}{2}(1-p)}(\varepsilon/a)^{-\frac{1}{2}(p+1)}(\varepsilon/a^2)\times$$

$$\times\{1+O(\mu^{-1})\}\{1+O(\varepsilon)\}\{1+O(a/\varepsilon)\} ,$$

and again, as $\mu \to \infty$ and $a \to 0$, ε fixed, the major term in $G_1'(\mu)$ above is the first. For $p = 1$,

$$G_1'(\mu) \sim -(p+1)^{1/2}e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}a^{-1} = -2^{1/2}e^{\frac{1}{2}\mu}\mu^{-1/2}a^{-1} .$$

For G_2, there exist constants $K_1(\varepsilon,A)$, $K_2(\varepsilon,A)$ such that

$$e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}K_1(\varepsilon,A) < G_2(\mu) < e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}K_2(\varepsilon,A) ,$$

$$e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}K_1(\varepsilon,A) < G_2'(\mu) < e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}K_2(\varepsilon,A) .$$

Clearly, G_1' dominates G_2'.

For G_3, $\sigma > A$, and so

$$G_3(\mu) = e^{\frac{1}{2}\mu} \int_A^\infty (\mu + \sigma)^{-2}\{\int_0^\sigma \frac{(a + \theta)^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta\}^{-1/2} d\sigma$$

$$= e^{\frac{1}{2}K^{-1}} \int_A^\infty (\mu + \sigma)^{-2}\{(\int_0^\infty - \int_\sigma^\infty) \frac{(a + \theta)^p}{(\mu + \theta)^{p+2}} e^{-(a+\theta)} d\theta\}^{-1/2} d\sigma$$

$$= e^{\frac{1}{2}K^{-1}} \int_A^\infty (\mu + \sigma)^{-2}\{(\int_a^\infty - \int_{a+\sigma}^\infty) \frac{\tau^p e^{-\tau}}{(\mu - a + \tau)^{p+2}} d\tau\}^{-1/2} d\sigma$$

(4.6) $$= e^{\frac{1}{2}K^{-1}} \int_A^\infty (\mu + \sigma)^{-2}\{(\int_0^A + \int_A^{a+\sigma} - \int_0^a) \frac{\tau^p e^{-\tau}}{(\mu - a + \tau)^{p+2}} d\tau\}^{-1/2} d\sigma$$

(4.7) $$= e^{\frac{1}{2}K^{-1}} \mu^{\frac{1}{2}p+1} \int_A^\infty (\mu+\sigma)^{-2}(\int_0^\infty \tau^p e^{-\tau} d\tau)^{-1/2} d\sigma\{1+O(\mu^{-1})\}\{1+O(a)\}\{1+O(A^p e^{-A})\} ,$$

where the O-terms may depend on A,

$$=(p!)^{-1/2} e^{\frac{1}{2}K^{-1}} \mu^{\frac{1}{2}p}\{1 + O(\mu^{-1})\}\{1 + O(a)\}\{1 + O(A^p e^{-A})\} .$$

In differentiating G_3, we must be careful, for formal differentiation of the leading term does not give the correct result. If we denote the expression in $\{....\}$ in (4.6) by $J(\sigma,\mu)$, then

$$G_3'(\mu) = - 2e^{\frac{1}{2}K^{-1}} \int_A^\infty (\mu + \sigma)^{-3}\{J(\sigma,\mu)\}^{-1/2} d\sigma$$

(4.8)

$$- \frac{1}{2} e^{\frac{1}{2}K^{-1}} \int_A^\infty (\mu + \sigma)^{-2}\{J(\sigma,\mu)\}^{-3/2}\{\frac{(a + \sigma)^p e^{-(a+\sigma)}}{(\mu + \sigma)^{p+2}} - \frac{a^p e^{-a}}{\mu^{p+2}}\} d\sigma .$$

In passing from (4.6) to (4.7), we saw that, for large μ, A,

$$J(\sigma,\mu) \sim p!\mu^{-(p+2)} ,$$

and so the first term on the right of (4.8) is $O(e^{\frac{1}{2}K^{-1}} \mu^{\frac{1}{2}p-1})$, which cannot balance

$G_1'(\mu)$. The term involving $(a+\sigma)^p$ is again

$$O\left(e^{\frac{1}{2}\kappa^{-1}}\mu^{\frac{3}{2}p+3}\int_A^\infty (\mu+\sigma)^{-(p+4)}\sigma^p e^{-\sigma}d\sigma\right) = O\left(e^{\frac{1}{2}\kappa^{-1}}\mu^{\frac{1}{2}p-1}\right),$$

but the term involving a^p is asymptotically

$$\frac{1}{2}\,e^{\frac{1}{2}\kappa^{-1}}(p!)^{-3/2}\mu^{\frac{1}{2}p+1}a^p\int_A^\infty (\mu+\sigma)^{-2}d\sigma = \frac{1}{2}\,e^{\frac{1}{2}\kappa^{-1}}(p!)^{-3/2}\mu^{\frac{1}{2}p}a^p\left(1+\frac{A}{\mu}\right)^{-1}.$$

For $G'(\mu) = 0$ we must have a balance between $G_1'(\mu)$ and $G_3'(\mu)$, and so, fixing e, A^{-1} as small as we please, and then letting $\mu \to \infty$, $a \to 0$, we have, for $p > 1$,

$$\frac{1}{2}\,(p+1)^{1/2}(p-1)e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}a^{-\frac{1}{2}(p+1)}\int_0^\infty \{(\phi+1)^{p+1}-1\}^{-1/2}d\phi$$

$$\sim \frac{1}{2}\,(p!)^{-3/2}e^{\frac{1}{2}\kappa^{-1}}\mu^{\frac{1}{2}p}a^p,$$

so that

(4.9) $$a^{\frac{1}{2}(3p+1)} \sim (p!)^{3/2}(p-1)(p+1)^{1/2}\left(\frac{1+\beta}{\gamma}\right)\int_0^\infty \{(\phi+1)^{p+1}-1\}^{-1/2}d\phi\ .$$

In the case $p = 1$, we have

$$(p+1)^{1/2}e^{\frac{1}{2}\mu}\mu^{\frac{1}{2}p-1}a^{-1} \sim \frac{1}{2}\,(p!)^{-3/2}e^{\frac{1}{2}\kappa^{-1}}\mu^{\frac{1}{2}p}a^p,$$

so that

(4.10) $$a \sim 2^{3/4}(1+\beta)^{1/2}\gamma^{-1/2}\ .$$

Finally, to show that the zero of $G'(\mu)$ is unique and simple, we have to verify that, in the relevant range for μ, $G''(\mu) > 0$. This is now a routine calculation, and we leave it to the reader.

5. THE CASE $p \neq 0$ WITH NON-ZERO BOUNDARY DATA

We now consider

$$v'' + \lambda(1 + \beta - v)^p e^{-\gamma/v} = 0 ,$$

with

$$v'(0) = 0, \quad v(1) = 1 ,$$

and (for physical reasons) we are interested in solutions for which $v < 1 + \beta$. With the same substitutions as in §2, this reduces to

$$Y'' + \lambda(1 + \beta - \alpha Y)^p e^{-\gamma/\alpha Y} = 0 ,$$

$$Y(0) = 1, \quad Y'(0) = 0, \quad Y(\alpha^{-1/2}) = \alpha^{-1}, \quad \alpha < 1 + \beta ,$$

and since Y is clearly non-increasing, we must have $\alpha > 1$. Then

$$\alpha^{-1/2} = (2\lambda)^{-1/2} \int_{\alpha^{-1}}^{1} \left(\int_{Y}^{1} (1 + \beta - \alpha t)^p e^{-\gamma/\alpha t} dt\right)^{-1/2} dY ,$$

or, with $\gamma = \alpha\mu$, $\gamma/(1 + \beta) < \mu < \gamma$,

$$\left(\frac{2\lambda}{\gamma}\right)^{1/2} = \mu^{-1/2} \int_{\mu/\gamma}^{1} \left(\int_{Y}^{1} \left(1 + \beta - \frac{\gamma t}{\mu}\right)^p e^{-\mu/t} dt\right)^{-1/2} dY .$$

With

$$K = (1 + \beta)/\gamma, \quad t = \mu/u, \quad Y = \mu/T ,$$

we have

$$\gamma^{1/2p}\left(\frac{2\lambda}{\gamma}\right)^{1/2} = \int_{\mu}^{\gamma} T^{-2}\left\{\int_{\mu}^{T} u^{-2}\left(K - \frac{1}{u}\right)^p e^{-u} du\right\}^{-1/2} dT .$$

With $u = \mu + \theta$, $T = \mu + \sigma$, we finally have

$$K^{\frac{1}{2}p}\gamma^{\frac{1}{2}p}\left(\frac{2\lambda}{\gamma}\right)^{1/2} = e^{\frac{1}{2}\mu} \int_{0}^{\gamma-\mu} (\mu + \sigma)^{-2}\left\{\int_{0}^{\sigma} \frac{(\mu + \theta - K^{-1})^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta\right\}^{-1/2} d\sigma .$$

Now define, for $\gamma/(1 + \beta) < \mu < \gamma$,

$$G^*(\mu) = e^{\frac{1}{2}\mu} \int_0^{\gamma-\mu} (\mu + \sigma)^{-2} \{\int_0^{\sigma} \frac{(\mu + \theta - K^{-1})^p}{(\mu + \theta)^{p+2}} e^{-\theta} d\theta\}^{-1/2} d\sigma \; .$$

__Theorem 6__. __For__ γ __sufficiently large__, β __fixed__, $K = (1 + \beta)/\gamma$, $G^{*\prime}(\mu)$ __has precisely two zeros in the range__ $\gamma/(1 + \beta) < \mu < \gamma$, __both simple. One occurs near the zero of__ $G(\mu)$, __the other asymptotically at__ $\mu = \gamma - 2 \log x_0$, __where__ x_0 __is as in Theorem 3__.

__Proof__. The proof of this need not be given in detail since it is in effect just a repetition of parts of the proofs of Theorems 3 and 5. If u is such that $\gamma - \mu \to \infty$ as $\gamma \to \infty$, then $G^*(\mu)$ can be analysed as $G(\mu)$ in Theorem 5. The result is that, in such a range of μ, $G^{*\prime}(\mu)$ has precisely one zero, and that simple, with the value of $a = \mu - K^{-1}$ satisfying (4.9) or (4.10). If μ is such that $\gamma - \mu = o(\gamma)$, and this clearly overlaps with the previous range of μ, then we can treat G^* as we did f_1 in Theorem 3. What the analysis there shows is that, to determine the asymptotic behaviour to the required degree of accuracy, we treat $\mu + \theta - K^{-1}$ as though it were $\mu - K^{-1}$, and $\mu + \theta$ and $\mu + \sigma$ as though they were μ. Then

$$G^*(\mu) \sim e^{\frac{1}{2}\mu} \mu^{\frac{1}{2}p-1} (\mu - K^{-1})^{-\frac{1}{2}p} \int_0^{\gamma-\mu} (\int_0^{\sigma} e^{-\theta} d\theta)^{-1/2} d\sigma$$

$$= e^{\frac{1}{2}\mu} \mu^{\frac{1}{2}p-1} (\mu - K^{-1})^{-\frac{1}{2}p} \int_0^{\gamma-\mu} (1 - e^{-\sigma})^{-1/2} d\sigma$$

$$= 2e^{\frac{1}{2}\mu} \mu^{\frac{1}{2}p-1} (\mu - K^{-1})^{-\frac{1}{2}p} \int_1^{\exp\{\frac{1}{2}(\gamma-\mu)\}} (x^2 - 1)^{-1/2} dx$$

$$= 2e^{\frac{1}{2}\mu} \mu^{\frac{1}{2}p-1} (\mu - K^{-1})^{-\frac{1}{2}p} \cosh^{-1}(e^{\frac{1}{2}\gamma}/e^{\frac{1}{2}\mu}) \; .$$

This is the same as the asymptotic expression for $f_1(\mu)$ except that μ^{-1} is replaced by $\mu^{\frac{1}{2}p-1} (\mu - K^{-1})^{-\frac{1}{2}p}$, and $\gamma e^{\frac{1}{2}\gamma}/\mu e^{\frac{1}{2}\mu}$ by $e^{\frac{1}{2}\gamma}/e^{\frac{1}{2}\mu}$. The latter pair are asymptotically the same when $\gamma - \mu$ is bounded, which is the range we are interested in, and the former pair play no part in determining the asymptotic position of μ since when we differentiate

these factors in f_1 or G^*, their derivatives do not contribute to the leading terms in f_1' or $G^{*\prime}$. Thus the final answer for G^* is asymptotically the same as that for f_1, as required.

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In catalysis theory there is interest in the number of solutions of the equation

$$v'' + \lambda(1 + \beta - v)^p e^{-\gamma/v} ,$$

with the boundary conditions

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ABSTRACT (cont.)

$$v'(0) = 0, \quad v(1) = 1 ,$$

the parameters λ, β, γ being all positive and p a non-negative integer. The paper answers this question when γ is large, which is the interesting situation physically, and although the treatment is somewhat different in the cases $p = 0$ and $p \neq 0$, the final answer is the same, that, given β, there exist two positive functions $\lambda_1(\gamma)$ and $\lambda_2(\gamma)$ such that the problem has one solution if $\lambda < \lambda_1(\gamma)$ or $\lambda > \lambda_2(\gamma)$, three solutions if $\lambda_1(\gamma) < \lambda < \lambda_2(\gamma)$, and two solutions if $\lambda = \lambda_1(\gamma)$ or $\lambda = \lambda_2(\gamma)$.

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